Stochastic variational method with noncentral forces

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Abstract

This paper extends the application of the stochastic variational method to noncentral interactions. Several examples are presented for three- and four-nucleon systems with realistic nuclear forces. The correlated Gaussians easily cope with the strong short range repulsion of the potential and the stochastic variational method efficiently selects the most important spin, isospin and orbital angular momentum components of the wave function. The examples confirm the usefulness and accuracy of the method.

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In a recent paper [1] we have shown that the stochastic variational method with correlated Gaussian basis (SVM) provides an accurate solution for various few-body systems. The applications of the SVM, however, were limited to central interactions so far [1–3]. The real challenge in nuclear few-body problems is the solution with a realistic nucleon-nucleon interaction including spin-orbit, tensor, etc. potentials. The application of the SVM for realistic interactions is, therefore, a stringent test of the usefulness of the method.

The SVM selects the most appropriate basis states in a trial and error procedure: various randomly generated trial states are tested and the usefulness of these states are judged from their contribution to the energy of the system. As it is a variational method, the choice of the functional form of the trial states greatly determines the accuracy and applicability of the method. We prefer the correlated Gaussians as trial functions, as these functions proved to be enormously accurate in few-body problems with zero orbital angular momentum. It is remarkable that the variational calculations with these functions give one of the most precise results up to date, for example, for the hydrogen molecular ion, the helium atom and the positronium molecule, reaching 13 digits accuracy [4]. Another advantage of the correlated Gaussian functions is that one can easily calculate their matrix elements [1] and one can easily extend the calculation to more than A=3,4 particle systems. These features make it especially interesting to test their applicability in few-nucleon systems with realistic forces.

The secret of the accuracy of the variational methods on the correlated Gaussian basis is the careful selection ("optimization") of the nonlinear parameters. In the SVM with central interaction these nonlinear parameters are the subject of the random test.

In nuclear physics the spin, isospin and orbital angular momentum dependence of the interaction is extremely important. To extend the application of the SVM for nuclear systems with realistic interactions, besides the previously applied random selection of the nonlinear parameters of the correlated Gaussians, a random selection of the spin and orbital components of the wave function is introduced.

The literature is very rich in papers devoted to few-nucleon problems [5–15]. For A=3 nuclei it is possible to include enough channels and an exact Faddeev calculation can be

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performed [12], but other methods (e.g., Variational Monte Carlo [14], Green Function Monte Carlo [5], Correlated Hyperspherical Harmonics [8], ATMS [15], or the Gaussian Variational Method (GVM) [9]) give essentially the same results. For A=4 nuclei some of these methods become too complicated, and the results of the existing calculations [5,8,10,14] agree only within a few hundreds keV. The development of other methods is therefore very important.

The purpose of this paper is to present a SVM calculation for the ^{3}H and ^{4}He nuclei with the interactions V6 (1, $\sigma \cdot \sigma$, $\tau \cdot \tau$, $\sigma \cdot \sigma \tau \cdot \tau$, S, S$\tau \cdot \tau$) and V8 (1, $\sigma \cdot \sigma$, $\tau \cdot \tau$, $\sigma \cdot \sigma \tau \cdot \tau$, S, S$\tau \cdot \tau$, $L \cdot S$, $L \cdot S \tau \cdot \tau$) and to compare with the results of other calculations in order to confirm the usefulness and accuracy of the SVM.

The trial function is defined in the following way:

$$\psi_{(LS)JMTM_T}(\mathbf{x}, A) = \mathcal{A}\{e^{-\frac{1}{2}\mathbf{x}A\mathbf{x}} [\theta_L(\mathbf{x})\chi_S]_{JM} \eta_{TM_T}\}, \tag{1}$$

where $\mathbf{x} = (\mathbf{x}_1, ..., \mathbf{x}_{N-1})$ is a set of relative (Jacobi) coordinates, the operator $\mathcal{A}$ is an antisymmetrizer, χ_{SM_S} is the spin function, and η_{TM_T} is the isospin function. The matrix A is an $(A-1) \times (A-1)$ matrix of the nonlinear variational parameters. The function $\theta_{LM_L}(\mathbf{x})$ represents the angular part of the wave function. It is taken as a vector coupled product of partial waves

$$\theta_{LM_L}(\mathbf{x}) = \left[\left[[Y_{l_1}(\mathbf{x_1})Y_{l_2}(\mathbf{x_2})]_{l_{12}} Y_{l_3}(\mathbf{x_3})\right] ...\right]_{LM_L}. \tag{2}$$

The spin and isospin functions are also successively coupled, for example

$$\chi_{SM_S} = \chi_{s_{12}s_{123}...SM_S} = [[[\chi_{\frac{1}{2}}\chi_{\frac{1}{2}}]_{s_{12}}\chi_{\frac{1}{2}}]_{s_{123}}...]_{SM_S} \tag{3}$$

For the triton, we used the partial wave channels with $(l_1, l_2)L$, $(l_1 + l_2 \leq 4, l_i \leq 2)$ and $L = 0, 1, 2$. For the alpha particle, all partial waves $((l_1, l_2)l_{12}, l_3)L$ satisfying the condition $l_1 + l_2 + l_3 \leq 4$, $l_i \leq 2$, $|l_1 - l_2| \leq l_{12} \leq l_1 + l_2$ and $L = 0, 1, 2$ have been tried. There are 3 spin and 2 isospin channels for the triton, and 6 spin and 2 isospin channels for the alpha particle. These channels are listed in Table II of ref. [1].

The basis setup of the SVM can be briefly described as follows : Let us assume that the dimension of the basis is $K - 1$.

(1) Generate $\mathcal{N}$ random candidates to find the Kth basis function:

(1a) Pick up a spin, isospin and partial wave channel randomly. (Some of the possibilities are listed in Table I.)

(1b) Select the nonlinear parameters randomly from a "physically" important interval.

(2) Calculate the ground state energy on the K basis states.

(3) Select the basis state which gave the lowest energy amongst the randomly generated trial functions and add it to the basis.

(4) Increase the dimension to $K + 1$.

In principle it would be more powerful to change all the K basis states randomly, but that requires repetitions of diagonalization of $K \times K$ matrices and becomes prohibitively computer time consuming. In the procedure (1)-(2)-(3)-(4) only one of the row (column) of the matrices changes, and there is no need for diagonalization to calculate the lowest eigenvalue [1]. A numerical optimatization of the basis would be an other option, but it is highly nontrivial. The reason is partly that number of nonlinear parameters is too large and partly that the channels (components of the wave functions with different quantum numbers) cannot be treated as continouos parameters and therefore the strategies of the numerical optimatizations can hardly be applied.

The main motivation for the random selection is that the number of channels and the nonlinear parameters are prohibitively large, therefore the calculation of all of the matrix elements and diagonalization including all potentially important basis states is out of the question. In the case of the alpha particle, for example, there are 12 spin-isospin channels and 32 partial wave channels even in our truncated partial wave expansion. The simplest choice of the nonlinear parameters of the Gaussian basis is to use only a diagonal matrix A. One may choose the diagonal elements as a geometric progression [9], for example. To reach good accuracy at least five terms for each of A_{11}, A_{22} and A_{33} have to be used, requiring $5^3 = 125$ functions in a given channel. The spin-isospin and space part, therefore, would result in a basis size of about ten thousands $(2 \times 125 \times 12 \times 32)$ in such a "direct" calculation for the alpha particle.

It is difficult to decide which channels are important and how many spatial functions are needed amongst the above mentioned numerous possibilities. The SVM automatically selects the important basis states through steps (1)-(2)-(3)-(4). The energy of the already selected states can be improved further: After reaching a given dimension, say K, one can stop the calculation and refine the nonlinear parameters. This fine tuning is done by repeating the steps (1b)-(2)-(3), that is, by changing the nonlinear parameters of one of the basis states which belongs to the already selected basis set. The nonlinear parameters are changed in the same spirit as before by randomly selecting the best. This is repeated for different basis states until the energy gain is less than 0.005 MeV. In this case we do not change the channels that are already selected and keep the dimension fixed. In the first stage of the calculation (steps (1)-(2)-(3)-(4)), the first $K-1$ basis states are kept frozen, and the best Kth basis state is selected with respect to them, so its selection is limited by the already chosen basis states. In the refining steps all of these states play active role again. Depending on the value of $\mathcal{N}$, these steps considerably improve the energy. The dimensions at the refining steps and the best energies obtained on these basis sizes are listed in Tables II and III.

The matrix elements were calculated as described in ref. [1]. To check the calculation we compared the numerical values of our matrix elements to those calculated by Kamimura [9]. The matrix elements agree in all digits.

To test the method we used two, from the point of view of spatial form, rather different interactions. The first, the Argonne potential (AV6 and AV8) [16], is a well-behaved smooth function. The second, the Reid potential (RV8) [17] is more singular and includes a linear combination of $\exp\{-\mu r^2\}/r^k$-type terms. The latter potential can certainly cause some problems. The AV6 potential includes only central and tensor components and serves as a good test case for the inclusion of noncentral forces. The AV6 potential has the same central and tensor components as the AV14 potential [16]. The AV6 and AV8 potentials are used without Coulomb potential, while in the case of the RV8 potential the Coulomb interaction is added.

To keep the number of nonlinear parameters low, we restricted the matrix A to be diagonal in one of the possible Jacobi-coordinate system. In the case of the three-nucleon system we have only one possibility of the Jacobi coordinate $((NN)+N)$, and for the alpha particle we will use $(3N)+N$ ("K") (and $(2N)+(2N)$-type ("H") Jacobi-coordinates. (Note that the basis function is fully antisymmetrized.) This choice is also dictated by physical intuitions as it is natural to consider ^{3}H$+p$, ^{3}He$+n$ and $d + d$-type partitions in the alpha particle. Test calculations show that this choice already gives satisfactory results.

As seen in Tables II and III, the convergence is relatively fast both for the triton and alpha particle with the AV6 and AV8 potentials, but in the case of the RV8 potential, due to its singular nature and stronger repulsive core, the convergence is slower. The result of the calculation does not improve by increasing the basis size further. In the case of the triton higher partial waves are not expected to give substantial contribution. In ref. [9] the authors included $l_1 + l_2 \leq 4$ partial waves for the AV14 potential but the energy changed by merely 0.002 MeV.

As the different channels are nonorthogonal, it is not trivial to calculate their weights. As a rough guide for their relative "importance", we list the most often selected channels in Table I. By using only these channels one gets about 0.5 MeV less binding for the alpha particle, so these channels alone already give a good approximation for the wave function.

The results of SVM and other calculations are compared in Tables IV and V. We show and compare the results not only for the energy but for the root mean square radius and average kinetic and potential energy. The results remain the same by repeating the calculations several times starting from different random values. The results of SVM and GFMC are very close to each other. Except for the case of the alpha particle with AV6, the results of SVM are always close to the GFMC, though the expectation values of the kinetic and the potential energies are somewhat different.

One can get good solution on relatively small basis dimensions. About 50 basis states for the triton and about 200 basis states for the alpha particle give fairly good binding energies. The energy of the alpha particle in the basis size of 100 is already within 0.5 MeV of its

final value.

Variational calculations were considered to be inappropriate to give accurate ground state energies for light nuclei, as they might not be able to reproduce the large cancellation between the kinetic and potential energy [7]. Our calculation shows that, with the careful optimization of the nonlinear variational parameters, this is not the case. We can obtain accurate energies even in the case of the RV8 potential. We note that the $L \cdot S$ term of the RV8 potential has been cut off at magnitude of 1 GeV in the GFMC calculation to reduce the statistical fluctuations caused by the 1/r singularity of the potential. To be consistent with this, we repeated the calculation with and without this cut off. We got 0.02 MeV less binding for the alpha particle with the modified potential, so the difference is essentially negligible.

Once we have a basis for a given potential, one naturally expects that the same basis may give fair ground state energy for other potentials of similar nature as well. We have checked if it is really the case. The basis optimized for the RV8 potential gives excellent results (within 100 keV) for AV6 and AV8 as well. Due to the singular nature and stronger repulsive core of RV8, however, the basis optimized for AV8 gives about 500 keV less binding for the alpha particle with RV8 than the basis optimized for RV8 itself. This result is still not so bad and can be easily improved by refining the nonlinear parameters. Therefore, one does not have to look for a new basis set for different interactions, but the same basis can be used for a given system with some "fine tuning" if necessary. The same is hopefully true for the other $((LS)^2, L^2$, etc.) part of the interaction: an already selected basis can be tailored to these additional terms, that is, instead of the steps (1)-(2)-(3)-(4), the several times faster refining steps (1b)-(2)-(3) can be used.

It is obviously important to calculate accurate binding energies of light nuclei with realistic forces. For example, the two-neutron separation energy of ^{6}He is about 1 MeV, so that a few hundreds keV less binding is thought to change its neutron "halo" structure significantly. One of the advantages of the SVM is that it is relatively easy to extend it to A=5, 6, 7 nucleon systems [1]. The low dimension of the bases required to solve the A=3,4

nucleon problems confirms that it is possible to treat larger nuclei with realistic forces with the SVM. The formalism and the computer code itself is general [1], so the applicability is mostly limited by the memory and speed of the available computer. The partial wave decomposition would not be appropriate for larger systems, but can be efficiently substituted by a simpler formalism [1]. This study is under way.

In summary, we have presented a stochastic variational solution for the triton and alpha particle with realistic nuclear forces. The wave function of these systems is a linear combination of components with different spin, isospin, orbital angular momentum and space parts. To find a good variational solution, one has to choose each part of the components with due care. The stochastic variational method attempts to collect the most important basis functions by randomly selecting the spin, isospin, orbital angular momentum and space parts. The fact that the results are in good agreement with those of the best calculations in the literature encourages the applications of the method for other cases, such as A=6 and 7 nuclei.

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[18] M. Viviani, A Kievsky and S. Rosati, private communication.

[19] W. Glöckle and H. Kamada, private communication. In the case of RV8 potential, Coulomb energy of 0.75 MeV is added. For the alpha particle with RV8, the calculation includes maximum two-body angular momentum j_{max} up to 3.

TABLES

TABLE I. The most frequently selected channels of the three- and four-nucleon systems.

$(l_1, l_2)L$	s_{12}	S	t_{12}
(0,0)0	0	1/2	1
(0,0)0	1	1/2	0
(2,0)2	1	3/2	0
(0,2)2	1	3/2	0
(2,2)0	1	1/2	0

$((l_1, l_2)l_{12}, l_3)L$	s_{12}	s_{123}	S	t_{12}	Jacobi
((0,0)0,0)0	0	1/2	0	1	H
((0,0)0,0)0	1	1/2	0	0	H
((0,0)0,0)0	0	1/2	0	1	K
((2,2)0,0)0	1	1/2	0	0	K
((2,2)0,0)0	1	1/2	0	0	H
((0,2)2,0)2	1	3/2	2	0	K
((0,2)2,0)2	1	3/2	2	0	H
((2,0)2,0)2	1	3/2	2	0	H
((1,1)2,0)2	1	3/2	2	1	K
((2,2)2,0)2	1	3/2	2	0	K

TABLE II. The convergence of energy (in MeV) for the triton.

K	AV6	AV8	RV8
25	-6.63	-7.36	-6.53
50	-7.04	-7.69	-7.41
75	-7.11	-7.74	-7.54
100	-7.15	-7.79	-7.59

TABLE III. The convergence of energy (in MeV) for the alpha particle.

K	AV6	AV8	RV8
100	-24.22	-25.15	-23.35
200	-24.90	-25.50	-24.15
300	-25.13	-25.60	-24.35
400	-25.25	-25.62	-24.49

TABLE IV. Energies (in MeV) and radii (in fm) of the triton by different methods and with different interactions. The probability P_L is given in %.

	SVM	GFMC	FY	VMC	CHH
AV6					
$\langle T \rangle$	44.8				
$\langle V_6 \rangle$	-51.9	$-52.0(3.00)$		$-43.7(1.0)$	
$\langle r^2 \rangle^{\frac{1}{2}}$	1.76	1.75(0.10)		1.95(0.03)	
P_S	91.2				
P_P	< 0.1				
P_D	8.7				
E	-7.15	$-7.22(0.12)$[a]	-7.15[a]	$-6.33(0.05)$[a]	
AV8					
$\langle T \rangle$	46.3				
$\langle V_6 \rangle$	-52.9				
$\langle V_{LS} \rangle$	-1.2				
$\langle r^2 \rangle^{\frac{1}{2}}$	1.75				
P_S	91.1				
P_P	< 0.1				
P_D	8.9				
E	-7.79		-7.79[d]		-7.79[c]
RV8					
$\langle T \rangle$	52.2	54.0(0.20)	52.2		
$\langle V \rangle$	-59.8	$-62.0(0.20)$	-59.8		
$\langle r^2 \rangle^{\frac{1}{2}}$	1.75	1.68(0.07)	1.76		
P_S	90.3				
P_P	< 0.1				
P_D	9.7				

| E | -7.59 | $-7.54(0.10)^{\text{b}}$ | -7.59^{b} | $-7.44(0.03)^{\text{e}}$ | -7.60^{c} |

[a]Ref. [5].

[b]Ref. [6].

[c]Ref. [18].

[d]Ref. [11].

[e]Ref. [14].

TABLE V. Energies (in MeV) and radii (in fm) of the alpha particle by different methods and with different interactions. The probability P_L is given in %.

	SVM	GFMC	FY	VMC	CHH
AV6					
$\langle T \rangle$	100.1				
$\langle V_6 \rangle$	-125.4	$-122.0(3.0)$		$-122.0(1.0)$	
$\langle r^2 \rangle^{\frac{1}{2}}$	1.49	1.50(0.04)		1.50(0.01)	
P_S	84.3				
P_P	0.5				
P_D	15.1				
E	-25.25	$-24.79(0.20)$[a]		$-22.75(0.01)$[a]	
AV8					
$\langle T \rangle$	98.8				
$\langle V \rangle$	-124.4	$-124.20(1.0)$			
$\langle V_6 \rangle$	-121.5				
$\langle V_{LS} \rangle$	-2.9				
$\langle r^2 \rangle^{\frac{1}{2}}$	1.50	1.51(0.01)			
P_S	85.5				
P_P	0.3				
P_D	14.2				
E	-25.62	$-25.75(0.02)$	-25.31[c]		-25.60[e]
RV8					
$\langle T \rangle$	111.7	109.2(0.20)			
$\langle V_6 \rangle$	-139.1	$-137.5(0.20)$			
$\langle V_{LS} \rangle$	2.1	2.45(0.23)			
$\langle V_{coul} \rangle$	0.75	0.71(0.02)			
$\langle r^2 \rangle^{\frac{1}{2}}$	1.51	1.53(0.02)			

P_S	84.1				
P_P	0.4				
P_D	15.5	15.5(0.20)			
E	-24.49	$-24.55(0.13)^{\text{b}}$	-23.79^{f}	-23.26^{d}	-23.9^{e}

[a]Ref. [5].

[b]Ref. [6].

[c]Ref. [11].

[d]Ref. [14].

[e]Ref. [18].

[f]Ref. [19].